What is claimed is:

1. A method of generating a reference library of composite spectra including the following steps:

(i) acquiring multiple independent spectra for a known chemical under multiple instrument conditions, each independent spectrum including an x and y axis;

(ii) renumbering the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap; and

(iii) generating a composite spectrum for the known chemical by aligning the x-axes of the independent spectra on a composite x-axis.

2. The method of claim 1, additionally including the step of storing the composite spectrum on a computer readable medium.

3. The method of claim 1, where the independent spectra are stored in an intermediate reference library and the remaining steps for creating the composite spectrum are performed, on demand, in response to inputs by a user regarding desired spectral conditions, renumbering and/or intervening spacing units.

4. The method of claim 1, where the independent spectra are obtained on a mass spectrometer, where the x-axes for the independent spectra represent the mass to charge ratio (m/z) and where the y-axes for the independent spectra represent the abundance of detected ions or normalized relative abundance.

5. The method of claim 4, where said mass spectrometer utilizes atmospheric pressure ionization (API) and collision induced dissociation (CID) fragmentation.

6. The method of claim 5, where said mass spectrometer is coupled to a liquid chromatograph (LC).

7. The method of claim 5, where said multiple predefined instrument conditions are different CID voltages.

8. The method of claim 5, where the mass spectrometer is tuned with one or more tuning compounds prior to acquiring the independent spectra.

9. A reference library of composite spectra created in the following manner:

(i) acquiring multiple independent spectra for a known chemical under multiple instrument conditions, each independent spectrum including an x and y axis;

(ii) renumbering the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap; and

(iii) generating a composite spectrum for the known chemical from said independent spectra by aligning the x-axes of the independent spectra on a composite x-axis.

10. The reference library of claim 9, where said library is stored on a computer readable medium.

11. The reference library of claim 9, where the independent spectra are stored in a database and the remaining steps for forming the reference library of composite spectra occur, on demand, in response to inputs by a user regarding desired spectral conditions, renumbering and/or intervening spacing units.

12. The reference library of claim 9, where the independent spectra are obtained on a mass spectrometer, where the x-axes for the independent spectra represent the mass to charge ratio (m/z) and where the y-axes for the independent spectra represent the abundance of detected ions or normalized relative abundance.

13. The reference library of claim 12, where said mass spectrometer utilizes atmospheric pressure ionization (API) and collision induced dissociation (CID) fragmentation.

14. The reference library of claim 13, where said mass spectrometer is coupled to a liquid chromatograph (LC).

15. The reference library of claim 13, where said multiple predefined instrument conditions are different CID voltages.

16. The reference library of claim 13, where the mass spectrometer is tuned with one or more tuning compounds prior to acquiring the multiple independent spectra.

17. A method of identifying an unknown chemical including the following steps:

(i) acquiring multiple independent spectra for an unknown chemical under multiple instrument conditions, each independent spectrum including an x and y axis;

(ii) renumbering the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap;

(iii) generating a composite spectrum for the unknown chemical from said independent spectra by aligning the x-axes of the independent spectra on a composite x-axis; and

(iv) comparing the composite spectrum of the unknown chemical to the composite spectra of one or more known chemicals.

18. The method of claim 17, where step (iv) compares the composite spectrum of the unknown chemical to the composite spectra of one or more known chemicals stored in a reference library.

19. The method of claim 17, where step (iv) compares the composite spectrum of the unknown chemical to the composite spectra of one or more known chemicals generated from a reference library that contains multiple independent spectra of known chemicals taken under multiple instrument conditions.

20. The method of claim 17, where the comparing step is performed by a pattern matching algorithm.

21. The method of claim 17, where the comparing step generates a probability factor quantifying the probability that the unknown chemical corresponds to a chemical represented by a composite spectrum in the reference library.

22. The method of claim 17, where said independent spectra are obtained on a mass spectrometer, where the x-axes for the independent spectra represent the mass to charge ratio (m/z) and where the y-axes for the independent spectra represent the abundance of detected ions or normalized relative abundance.

23. The method of claim 22, where said mass spectrometer utilizes atmospheric pressure ionization (API) and collision induced dissociation (CID) fragmentation.

24. The method of claim 23, where said mass spectrometer is coupled to a liquid chromatograph (LC).

25. The method of claim 23, where said multiple predefined instrument conditions are different CID voltages.

26. The method of claim 23, where the mass spectrometer is tuned with one or more tuning compounds prior to acquiring the multiple independent spectra.

27. A computer readable medium, said computer readable medium including instructions to cause a computer to perform the following functions:

(i) receive multiple independent spectra for an unknown chemical obtained under multiple instrument conditions, each spectra having an x and y axis;

(ii) renumber the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap;

(iii) generate a composite spectrum for the unknown chemical from said independent spectra by aligning the x-axes of the independent spectra on a composite x-axis; and

(iv) compare the composite spectrum of the unknown chemical to the composite spectra of one or more known chemicals.

28. The computer readable medium of claim 27, which additionally includes a reference library of composite spectra for known chemicals.

29. The computer readable medium of claim 27, which additionally includes a library of individual spectra for known chemicals and instructions to cause a computer to derive a reference library of composite spectra from said library of individual spectra.

30. The computer readable medium of claim 27, which additionally includes instructions to cause a computer to generate a probability factor quantifying the probability that the unknown chemical corresponds to a known chemical.

31. The computer readable medium of claim 27, where step (iv) utilizes a pattern matching algorithm.

32. A device for identifying an unknown chemical including the following components:

(i) a spectrometer;

(ii) a computer;

(iii) a reference library of composite spectra generated by -

(a) acquiring multiple independent spectra for a known chemical compound under multiple predefined instrument conditions, each independent spectra including an x and y axis,

(b) renumbering the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap, and

(c) generating a composite spectrum for the known chemical compound from said independent spectra by aligning the x-axes of the independent spectra on a composite x-axis; and

(iii) a computer readable medium including instructions to cause a computer to perform the following functions –

(a) receive multiple independent spectra for an unknown chemical taken under multiple conditions, each of the spectra having an x and y axis,

(b) renumber the units on the x-axis of at least one of the independent spectra so that the x-axes of the independent spectra do not perfectly overlap,

(c) generate a composite spectrum for the unknown chemical from said independent spectra by aligning the x-axes of the independent spectra on a composite x-axis, and

(d) compare the composite spectrum of the unknown chemical to the composite spectra of known chemical compounds stored in the reference library.